

Lionel Perrin

List of Publications by Year in descending order

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78
papers

2,786
citations

172386

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92
docs citations

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times ranked

2880
citing authors

#	ARTICLE	IF	CITATIONS
1	Computed Ligand Electronic Parameters from Quantum Chemistry and Their Relation to Tolman Parameters, Lever Parameters, and Hammett Constants. <i>Inorganic Chemistry</i> , 2001, 40, 5806-5811.	1.9	233
2	Hydrogen for Fluorine Exchange in C ₆ F ₆ and C ₆ F ₅ H by Monomeric [1,3,4-(Me ₃ C) ₃ C ₅ H ₂] ₂ CeH: Δ Experimental and Computational Studies. <i>Journal of the American Chemical Society</i> , 2005, 127, 279-292.	6.6	190
3	Scope and Challenge of Computational Methods for Studying Mechanism and Reactivity in Homogeneous Catalysis. <i>ACS Catalysis</i> , 2019, 9, 6803-6813.	5.5	145
4	Theoretical and Experimental Studies on the Carbon Nanotube Surface Oxidation by Nitric Acid: Interplay between Functionalization and Vacancy Enlargement. <i>Chemistry - A European Journal</i> , 2011, 17, 11467-11477.	1.7	93
5	Hydrogen for Fluorine Exchange in CH ₄ -x F _x by Monomeric [1,2,4-(Me ₃ C) ₃ C ₅ H ₂] ₂ CeH: Δ Experimental and Computational Studies. <i>Journal of the American Chemical Society</i> , 2005, 127, 7781-7795.	6.6	91
6	$\hat{\Gamma}^3$ Agostic C $\hat{\Gamma}$ H or $\hat{\Gamma}^2$ agostic Si $\hat{\Gamma}$ C bonds in La{CH(SiMe ₃) ₂ } ₃ ? A DFT study of the role of the ligand. <i>New Journal of Chemistry</i> , 2003, 27, 121-127.	1.4	88
7	Bis(allyl)calcium. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 5715-5719.	7.2	81
8	Control of peptide nanotube diameter by chemical modifications of an aromatic residue involved in a single close contact. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 7679-7684.	3.3	81
9	A DFT Study of SiH ₄ Activation by Cp ₂ LnH. <i>Inorganic Chemistry</i> , 2002, 41, 4355-4362.	1.9	75
10	Elucidation of the Self-Assembly Pathway of Lanreotide Octapeptide into $\hat{\Gamma}^2$ -Sheet Nanotubes: Role of Two Stable Intermediates. <i>Journal of the American Chemical Society</i> , 2010, 132, 4230-4241.	6.6	75
11	DFT study of CH ₄ activation by d ⁰ Cl ₂ LnZ (Z = H, CH ₃) complexes. <i>Dalton Transactions RSC</i> , 2002, , 534-539.	2.3	74
12	Mono-, Di-, and Trianionic $\hat{\Gamma}^2$ -Diketiminato Ligands: Δ A Computational Study and the Synthesis and Structure of [(YbL) ₃ (THF)], L = [{N(SiMe ₃)C(Ph)} ₂ CH]. <i>Journal of the American Chemical Society</i> , 2003, 125, 10790-10791.	6.6	71
13	Olefin Epoxidation by H ₂ O ₂ /MeCN Catalysed by Cyclopentadienyloxidotungsten(VI) and Molybdenum(VI) Complexes: Experiments and Computations. <i>Chemistry - A European Journal</i> , 2010, 16, 9572-9584.	1.7	71
14	Remote functionalization of hydrocarbons with reversibility enhanced stereocontrol. <i>Chemical Science</i> , 2015, 6, 2770-2776.	3.7	65
15	Some structural and electronic properties of MX ₃ (M = Ln, Sc, Y, Ti ⁺ , Zr ⁺ , Hf ⁺ ; X = H, Me, Hal, NH ₂) from DFT calculations. <i>Faraday Discussions</i> , 2003, 124, 25-39.	1.6	59
16	Deciphering the Mechanism of Coordinative Chain Transfer Polymerization of Ethylene Using Neodymocene Catalysts and Dialkylmagnesium. <i>ACS Catalysis</i> , 2016, 6, 851-860.	5.5	50
17	Insertion of Pyridine into the Calcium Allyl Bond: Regioselective 1,4-Dihydropyridine Formation and C $\hat{\Gamma}$ H Bond Activation. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 7795-7798.	7.2	46
18	New perspectives in organolanthanide chemistry from redox to bond metathesis: insights from theory. <i>Chemical Society Reviews</i> , 2016, 45, 2516-2543.	18.7	44

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19	Are the Carbon Monoxide Complexes of Cp ₂ M (M = Ca, Eu, or Yb) Carbon or Oxygen Bonded? An Answer from DFT Calculations. <i>Journal of the American Chemical Society</i> , 2002, 124, 5614-5615.	6.6	43
20	CYTOCHROME P450-MEDIATED OXIDATION OF GLUCURONIDE DERIVATIVES: EXAMPLE OF ESTRADIOL-17 β -GLUCURONIDE OXIDATION TO 2-HYDROXY-ESTRADIOL-17 β -GLUCURONIDE BY CYP 2C8. <i>Drug Metabolism and Disposition</i> , 2005, 33, 466-473.	1.7	43
21	On the Initiation Mechanism of Syndiospecific Styrene Polymerization Catalyzed by Single-Component <i>ansa</i> -Lanthanidocenes. <i>Chemistry - A European Journal</i> , 2009, 15, 3773-3783.	1.7	42
22	Structural Role of Counterions Adsorbed on Self-Assembled Peptide Nanotubes. <i>Journal of the American Chemical Society</i> , 2012, 134, 723-733.	6.6	41
23	Isoselective Styrene Polymerization Catalyzed by <i>ansa</i> -Bis(indenyl) Allyl Rare Earth Complexes. Stereochemical and Mechanistic Aspects. <i>Macromolecules</i> , 2011, 44, 3312-3322.	2.2	40
24	Chemoselectivity in σ bond activation by lanthanocene complexes from a DFT perspective: reactions of Cp ₂ LnR (R = CH ₃ , H, SiH ₃) with SiH ₄ and CH ₃ -SiH ₃ . <i>New Journal of Chemistry</i> , 2007, 31, 549-555.	1.4	37
25	Ethylene- <i>trans</i> -Butadiene Copolymerization by Neodymocene Complexes: A Ligand Structure/Activity/Polymer Microstructure Relationship Based on DFT Calculations. <i>ACS Catalysis</i> , 2016, 6, 1028-1036.	5.5	37
26	A Joint Experimental/Theoretical Investigation of the Statistical Olefin/Conjugated Diene Copolymerization Catalyzed by a Hemi- <i>ansa</i> -Lanthanidocene [(Cp*)(BH ₄)LnR]. <i>Chemistry - A European Journal</i> , 2010, 16, 11376-11385.	1.7	34
27	DFT Investigation of the Tacticity Control during Styrene Polymerization Catalyzed by Single-Component Allyl <i>ansa</i> -Lanthanidocenes		

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37	Qualitative Estimation of the Single-Electron Transfer Step Energetics Mediated by Samarium(II) Complexes: A SOMO-LUMO Gap Approach. <i>Inorganic Chemistry</i> , 2014, 53, 3427-3433.	1.9	24
38	Preparation and Reactivity of Acyclic Chiral Allylzinc Species by a Zinc-Brook Rearrangement. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 6057-6061.	7.2	24
39	High Glass-Transition Temperature Polymer Networks Harnessing the Dynamic Ring Opening of Pinacol Boronates. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 12216-12222.	7.2	24
40	Straightforward Synthesis of β -Bromopenta-2,4-dienitrile and Its Reactivity Towards Terminal Alkynes: A Direct Access to Diene and Benzofulvene Scaffolds. <i>Chemistry - A European Journal</i> , 2015, 21, 6042-6047.	1.7	21
41	Preliminary Theoretical Insights into Sml ₂ -Mediated Reactions: Activation of Ketones in THF. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 4042-4049.	1.0	19
42	Theoretical treatment of one electron redox transformation of a small molecule using f-element complexes. <i>Dalton Transactions</i> , 2014, 43, 12124-12134.	1.6	19
43	Two [1,2,4-(Me) ₃ C] ₃ C ₅ H ₂ CeH Molecules are Involved in Hydrogenation of Pyridine to Piperidine as Shown by Experiments and Computations. <i>Inorganic Chemistry</i> , 2014, 53, 6361-6373.	1.9	19
44	An electrochemical and DFT study on selected β^2 -diketiminato metal complexes. <i>Dalton Transactions</i> , 2006, , 2591-2596.	1.6	18
45	A DFT study of conjugated dienes polymerisation catalyzed by [Cp*ScR] ⁺ : insights into the propensity for cis-1,4 insertion. <i>Chemical Communications</i> , 2010, 46, 2965.	2.2	17
46	Lanthanide Complexes: Electronic Structure and H-H, C-H, and Si-H Bond Activation from a DFT Perspective. <i>ACS Symposium Series</i> , 2004, , 116-133.	0.5	16
47	Probing the stereo-electronic properties of cationic rhodium complexes bearing chiral diphosphine ligands by ¹⁰³ Rh NMR. <i>Magnetic Resonance in Chemistry</i> , 2010, 48, 848-856.	1.1	16
48	Dialkenylmagnesium Compounds in Coordinative Chain Transfer Polymerization of Ethylene. Reversible Chain Transfer Agents and Tools To Probe Catalyst Selectivities toward Ring Formation. <i>Organometallics</i> , 2018, 37, 1546-1554.	1.1	16
49	A DFT Study of Stannane Dehydrocoupling Catalyzed by Cp ₂ LaH. <i>Organometallics</i> , 2006, 25, 3143-3151.	1.1	15
50	Development of a Modified Julia Olefination of Imides for the Synthesis of Alkaloids. <i>European Journal of Organic Chemistry</i> , 2016, 2016, 2944-2953.	1.2	15
51	The role of H ₂ O in the electron transfer-activation of substrates using Sml ₂ : insights from DFT. <i>Dalton Transactions</i> , 2016, 45, 3706-3710.	1.6	15
52	Iodine-Transfer Polymerization (ITP) of Ethylene and Copolymerization with Vinyl Acetate. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 19304-19310.	7.2	15
53	Facile Interconversion of [Cp ₂ (Cl)Hf(SnH ₃)] and [Cp ₂ (Cl)Hf(η^4 -H)SnH ₂]: DFT Investigations of Hafnocene Stannyl Complexes as Masked Stannylenes. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 1816-1819.	7.2	14
54	Reversible 1,4-Insertion of Pyridine Into a Highly Polar Metal-Carbon Bond: Effect of the Second Metal. <i>Chemistry - A European Journal</i> , 2012, 18, 6448-6452.	1.7	14

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55	Synthesis and biological evaluation of tetrahydro[1,4]diazepino[1,2-a]indol-1-ones as cyclin-dependent kinase inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2014, 83, 617-629.	2.6	14
56	Identification of a Transient but Key Motif in the Living Coordinative Chain Transfer Cyclocopolymerization of Ethylene with Butadiene. <i>ACS Catalysis</i> , 2019, 9, 9298-9309.	5.5	14
57	Mechanistic insights into $\hat{\text{I}}^2$ -oxygen atom transfer in olefinepoxidation mediated by W(vi) complexes and H ₂ O ₂ . <i>Dalton Transactions</i> , 2012, 41, 1131-1133.	1.6	13
58	Modelling and Rationalizing Organometallic Chemistry with Computation: Where Are We?. <i>Structure and Bonding</i> , 2015, , 1-37.	1.0	13
59	Exploring the Conformation of Mixed <i>Cis</i> and <i>Trans</i> $\hat{\text{I}}^{\pm}$, $\hat{\text{I}}^2$ -Oligopeptoids: A Joint Experimental and Computational Study. <i>Journal of Organic Chemistry</i> , 2018, 83, 6382-6396.	1.7	13
60	Stereoselective Synthesis of Enantiopure Cycloalkylglycines by 1,3-Dipolar Cycloaddition of a Chiral Nitron to Cycloalkenes. <i>European Journal of Organic Chemistry</i> , 2014, 2014, 6017-6024.	1.2	11
61	Experimental and DFT Computational Study of $\hat{\text{I}}^2$ -Me and $\hat{\text{I}}^2$ -H Elimination Coupled with Proton Transfer: From Amides to Enamides in Cp* ₂ MX (M = La, Ce). <i>Organometallics</i> , 2017, 36, 97-108.	1.1	11
62	Design of selective divalent chain transfer agents for coordinative chain transfer polymerization of ethylene and its copolymerization with butadiene. <i>Polymer Chemistry</i> , 2022, 13, 1970-1977.	1.9	11
63	Computational insights into carbon-carbon homocoupling reactions mediated by organolanthanide(III) complexes. <i>Dalton Transactions</i> , 2014, 43, 4520.	1.6	10
64	Metabolism of N-methylamide by cytochrome P450s. <i>FEBS Journal</i> , 2011, 278, 2167-2178.	2.2	9
65	Metabolism of Phenylahistin Enantiomers by Cytochromes P450: A Possible Explanation for Their Different Cytotoxicity. <i>Drug Metabolism and Disposition</i> , 2008, 36, 2381-2392.	1.7	8
66	Monocationic Bis-Alkyl and Bis-Allyl Yttrium Complexes: Synthesis, ⁸⁹ Y NMR Characterization, Ethylene or Isoprene Polymerization, and Modeling. <i>Organometallics</i> , 2021, 40, 218-230.	1.1	8
67	Ene/Diene Copolymerization Catalyzed by Cationic Sc and Gd d ⁰ Metal Complexes: Speciation, Ion Pairing, and Selectivity from a Computational Perspective. <i>ACS Catalysis</i> , 2020, 10, 12359-12369.	5.5	6
68	Salt-Enhanced Oxidative Addition of Iodobenzene to Pd: An Interplay Between Cation, Anion, and Pd-Pd Cooperative Effects. <i>Inorganic Chemistry</i> , 2022, 61, 7935-7944.	1.9	6
69	Iodine-Transfer Polymerization (ITP) of Ethylene and Copolymerization with Vinyl Acetate. <i>Angewandte Chemie</i> , 2020, 132, 19466-19472.	1.6	5
70	Block Copolymers Based on Ethylene and Methacrylates Using a Combination of Catalytic Chain Transfer Polymerisation (CCTP) and Radical Polymerisation. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 25356-25364.	7.2	5
71	Intramolecular hydrogen bonding as a determinant of the inhibitory potency of N-unsubstituted imidazole derivatives towards mammalian hemoproteins. <i>Metallomics</i> , 2009, 1, 148-156.	1.0	4
72	Water-soluble, heterometallic chalcogenide oligomers as building blocks for functional films. <i>Inorganic Chemistry Frontiers</i> , 2016, 3, 689-701.	3.0	3

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73	Preparation of monopodal and bipodal aluminum surface species by selective protonolysis of highly reactive [AlH ₃ (NMe ₂ Et)] on silica. Dalton Transactions, 2017, 46, 11547-11551.	1.6	3
74	Cationic Phenoxyimine Complexes of Yttrium: Synthesis, Characterization, and Living Polymerization of Isoprene. Organometallics, 2022, 41, 2106-2118.	1.1	3
75	Coordinative chain transfer copolymerization of ethylene and styrene using an <i>ansa</i> -bis(fluorenyl) neodymium complex and dialkylmagnesium. Polymer Chemistry, 2018, 9, 3262-3271.	1.9	2
76	A Career in Catalysis: Odile Eisenstein. ACS Catalysis, 2019, 9, 10375-10388.	5.5	2
77	Relating circular dichroism to atomic structure by means of MD simulations and computed CD spectra with α -peptoids as an example. Physical Chemistry Chemical Physics, 2020, 22, 13192-13200.	1.3	2
78	Block copolymers based on ethylene and methacrylates using a combination of catalytic chain transfer polymerisation (CCTP) and radical polymerization. Angewandte Chemie, 2021, 133, 25560.	1.6	0